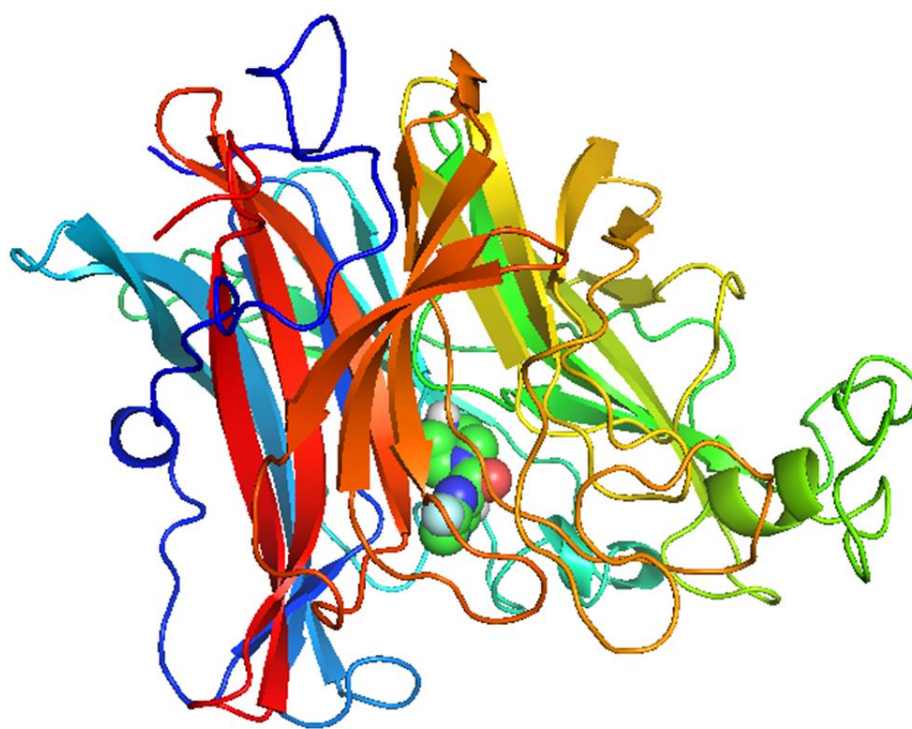
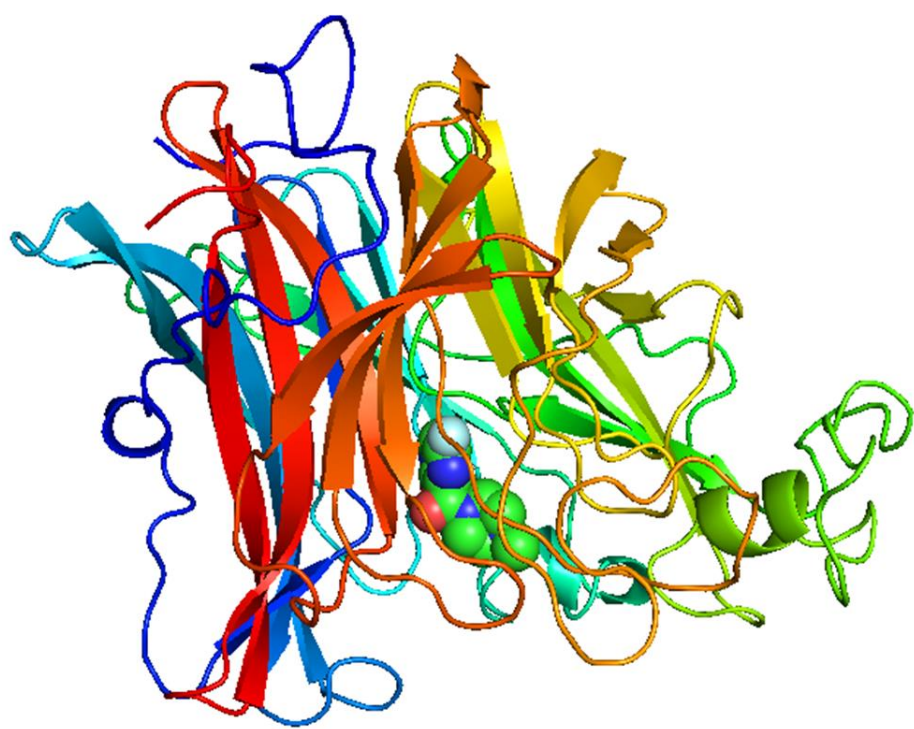


Supplementary Material

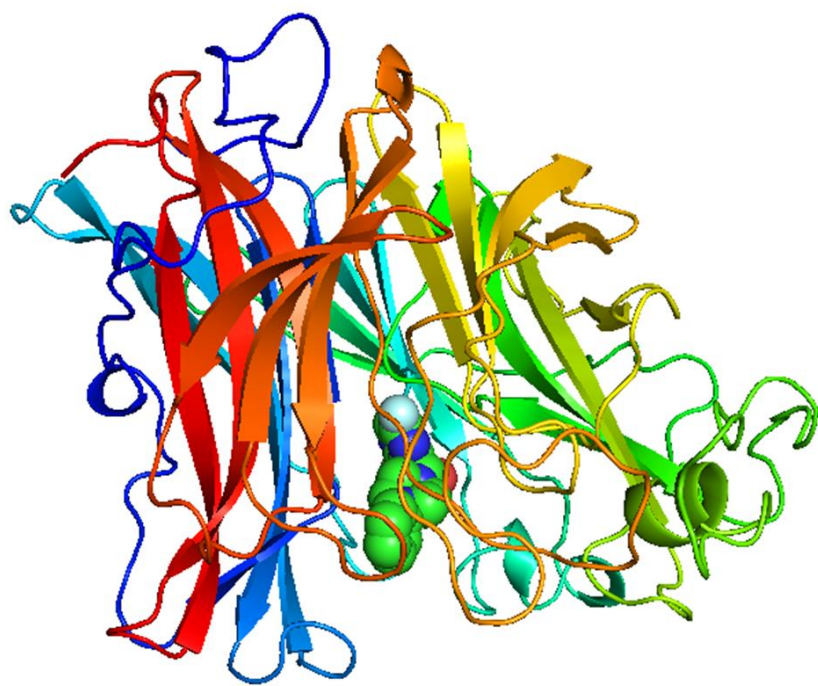
Fig. S1. 3D view of the binding conformations of molecule at the active site of the protein



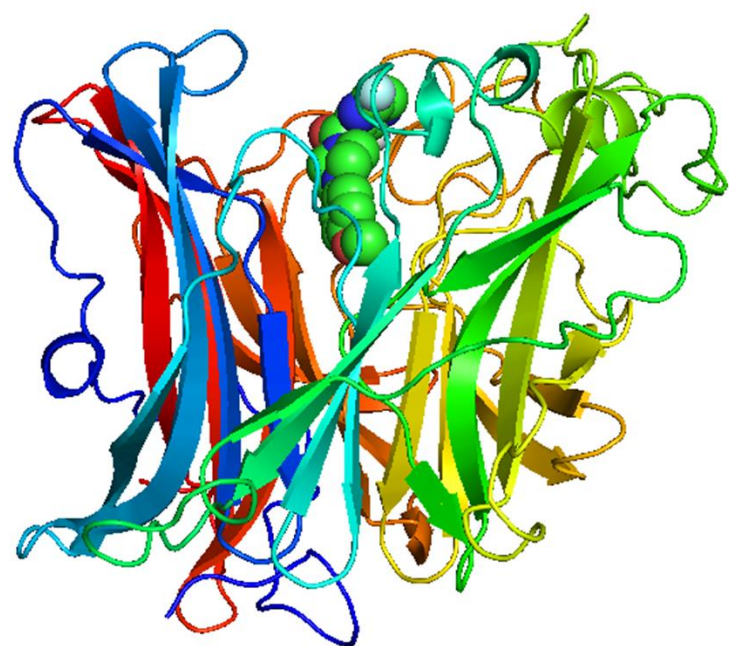
F1



F2



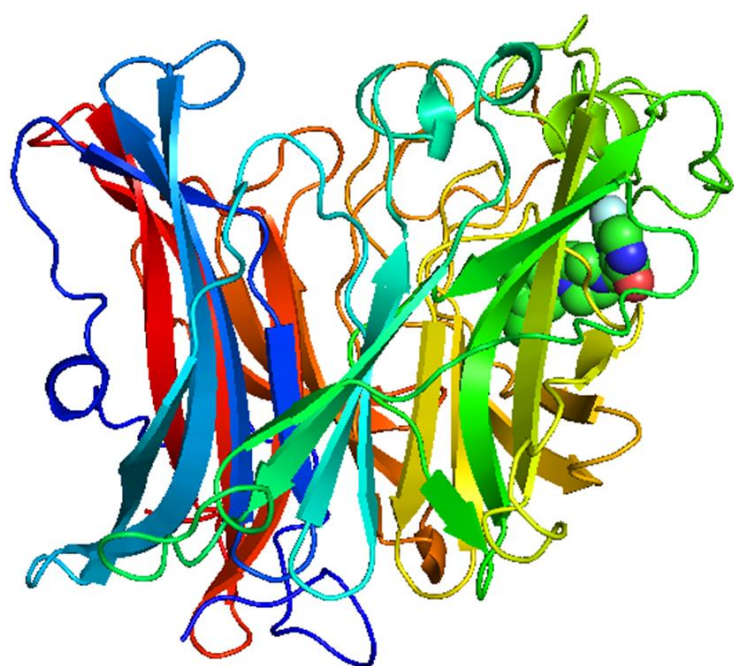
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F4



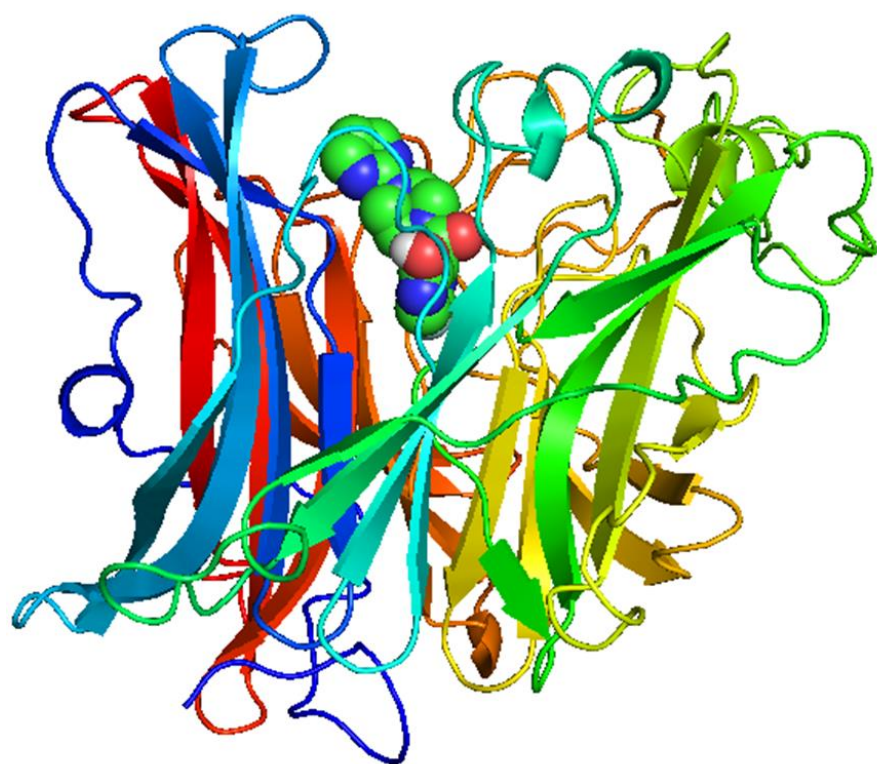
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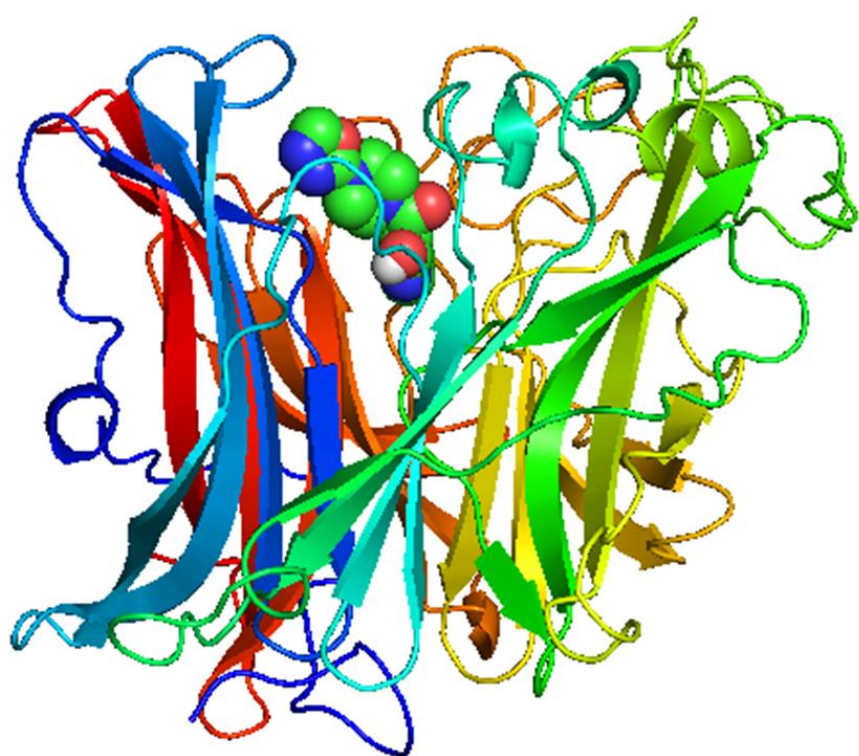
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F7



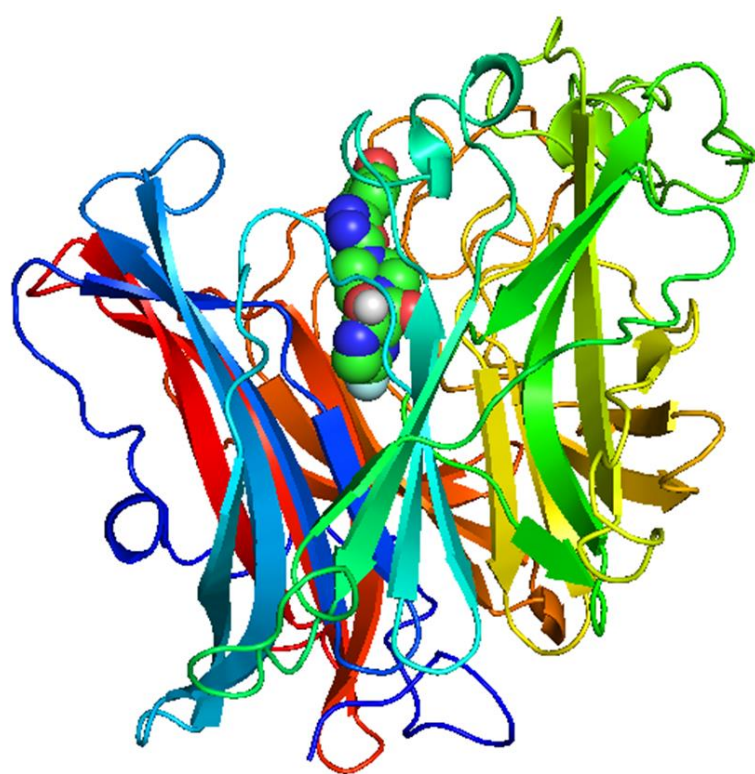
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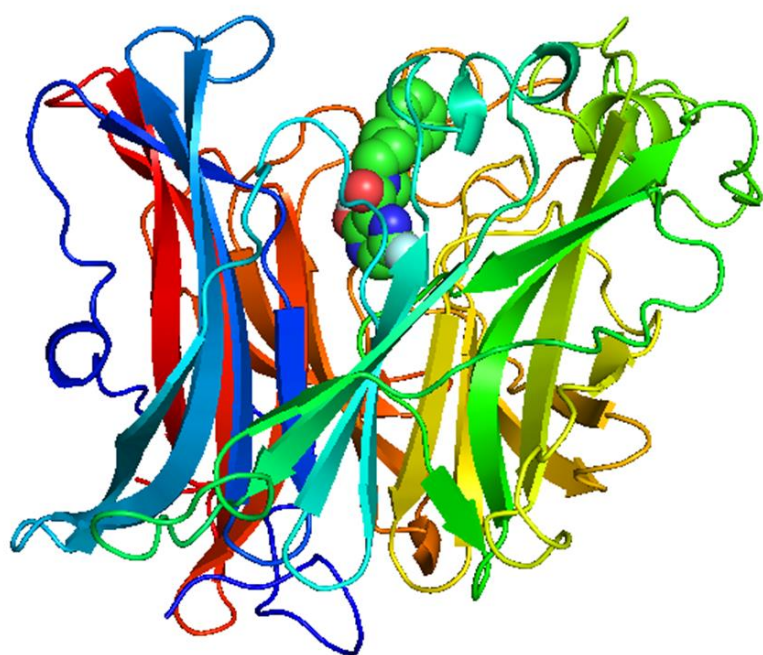
F9



F13

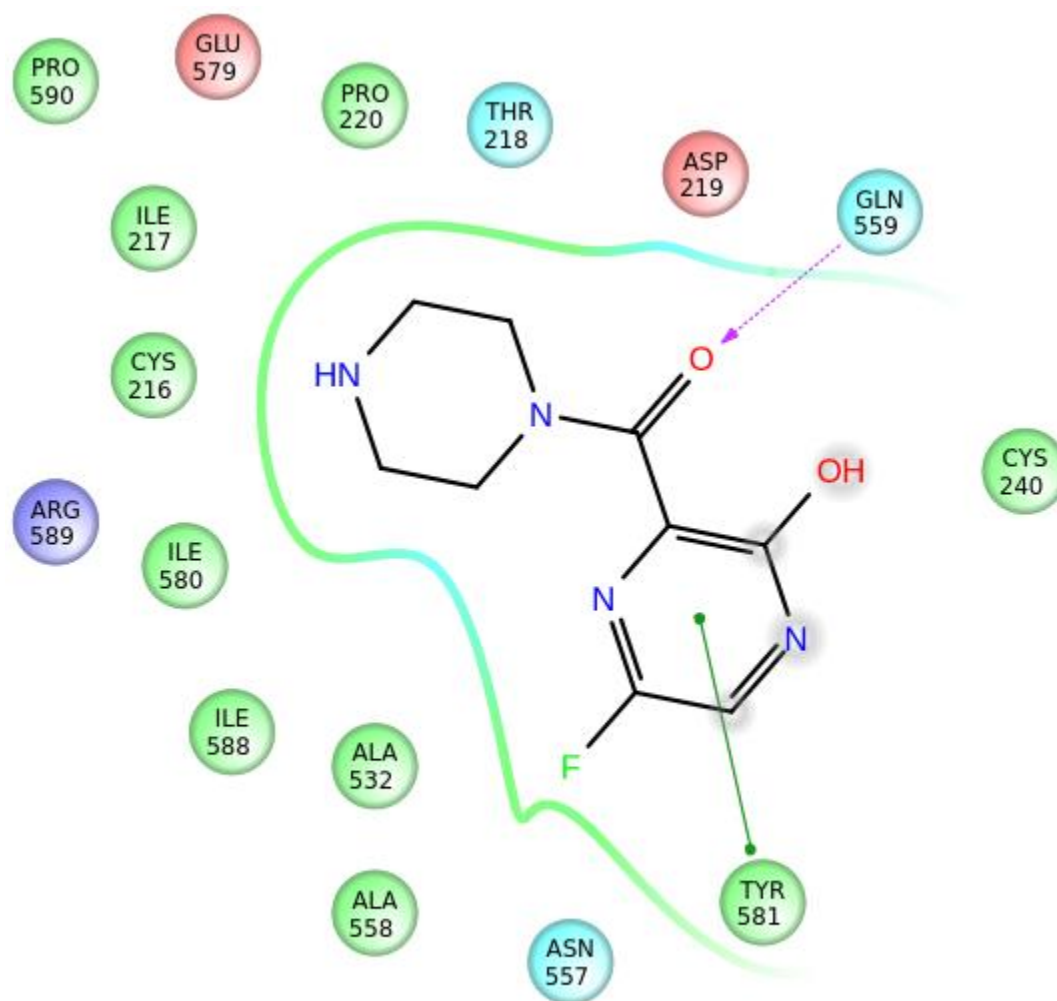


F14

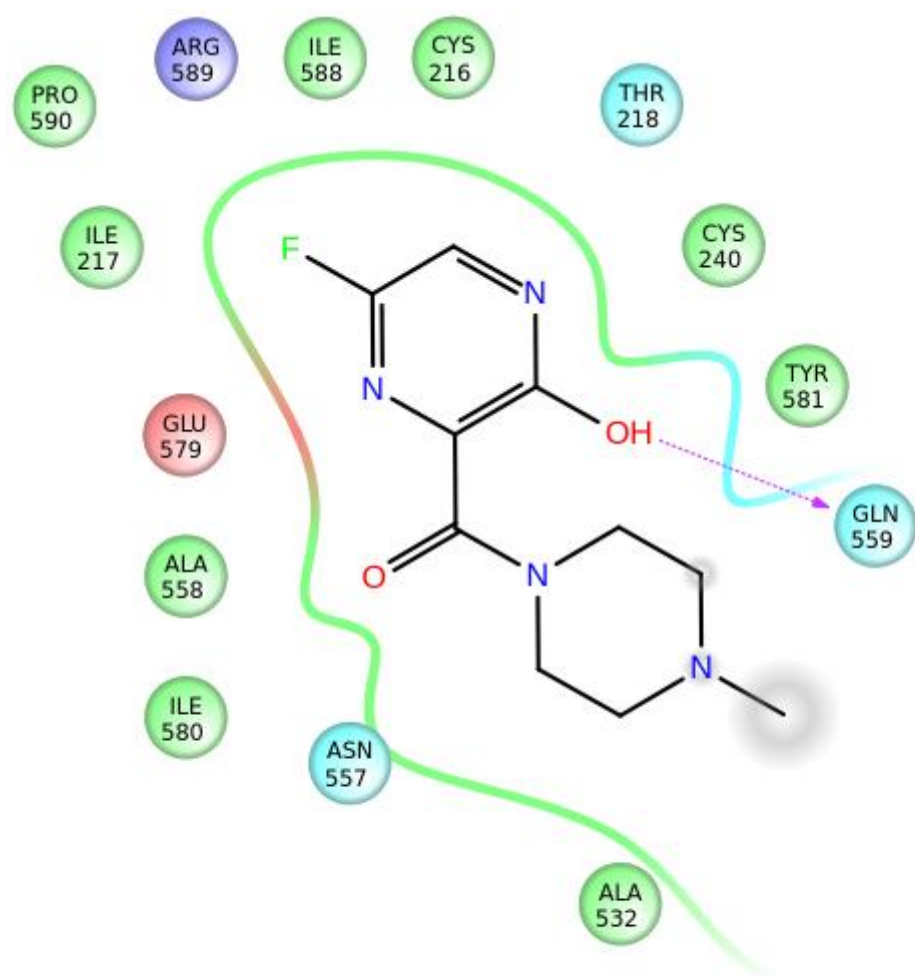


F15

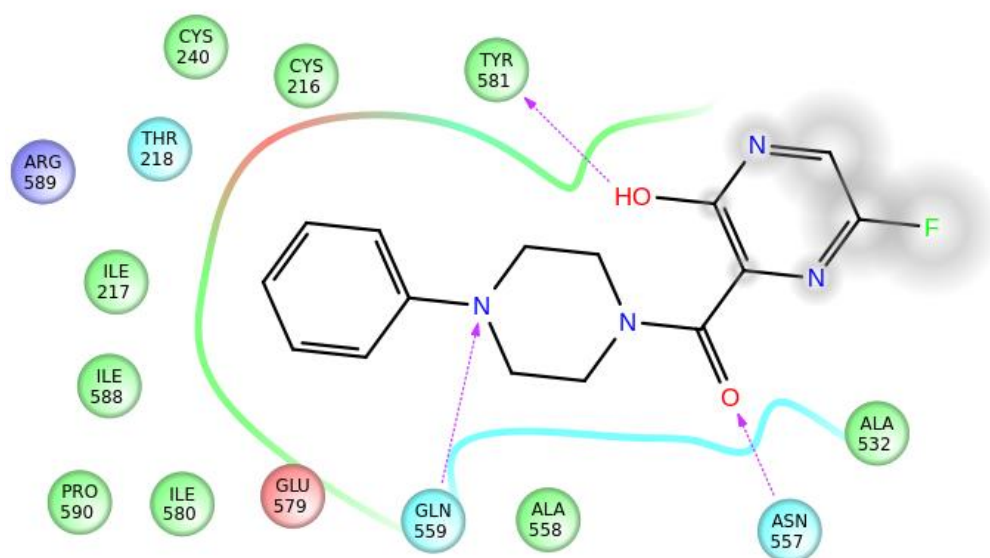
Fig S2. Interactions made by the molecules with the targeted protein (3D11) analysed using Ligplot



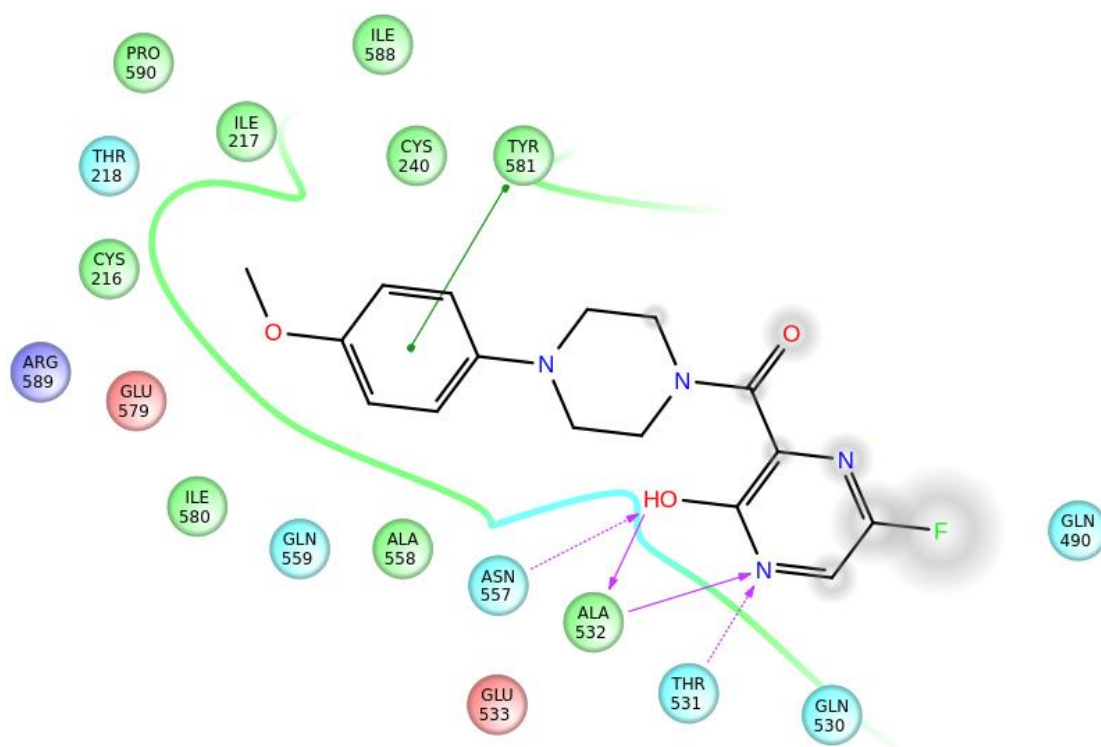
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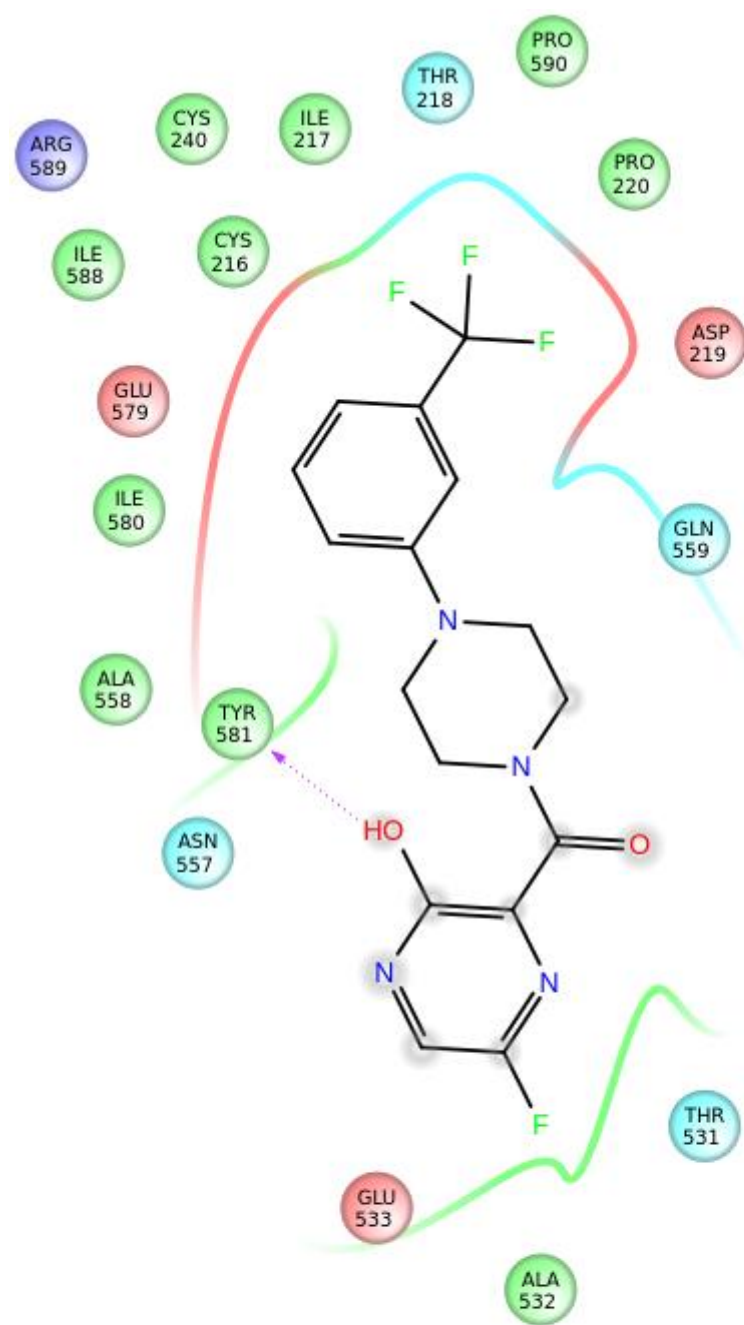
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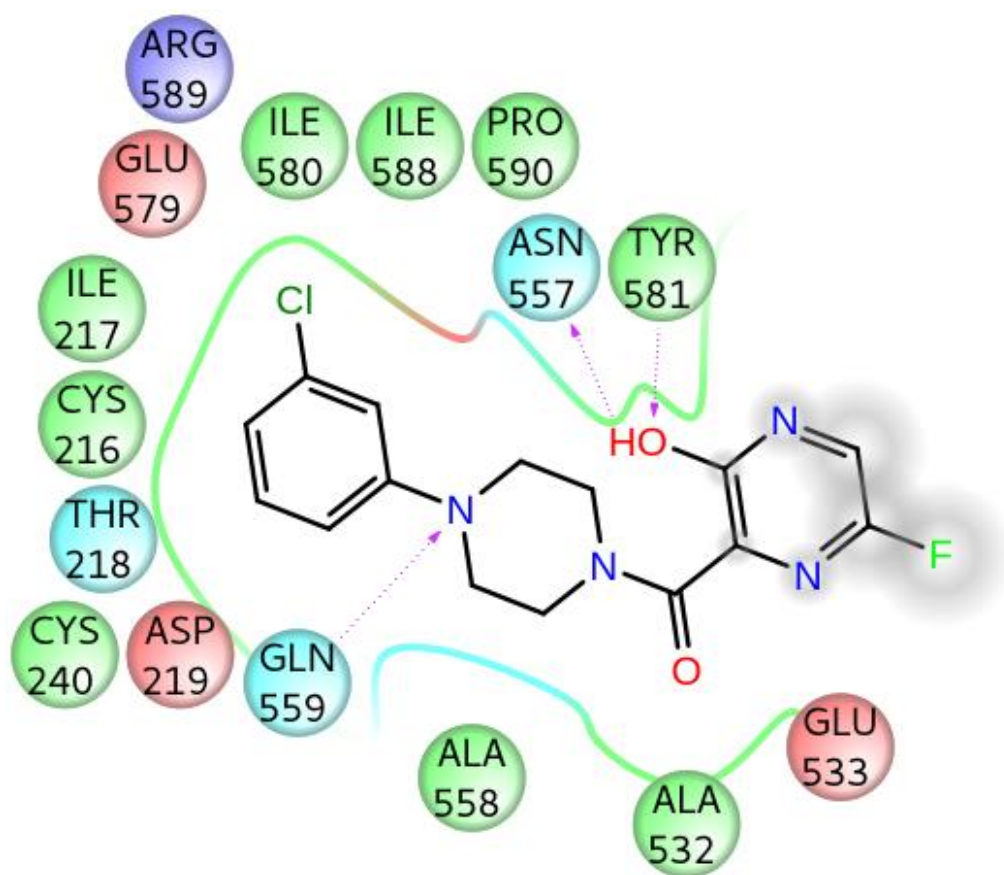
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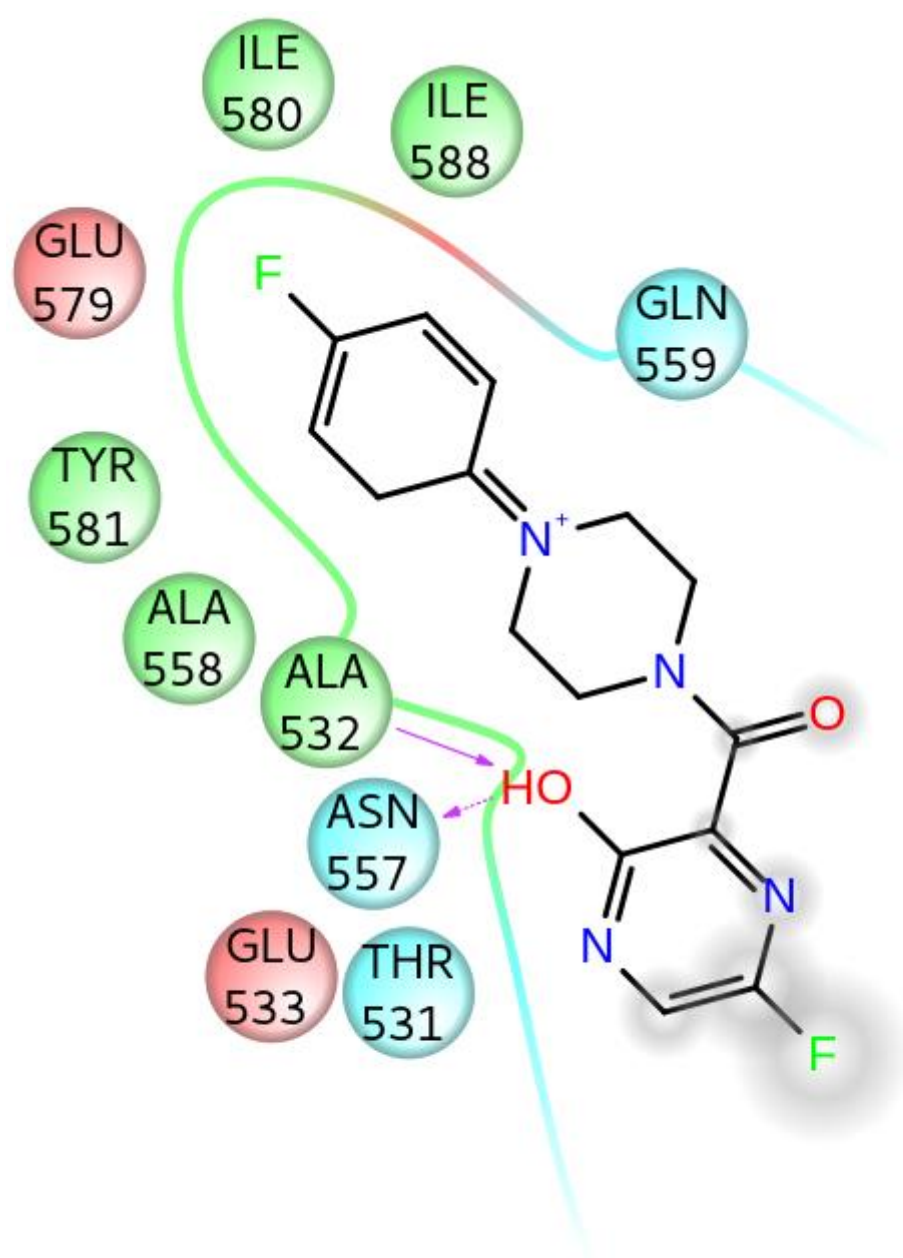
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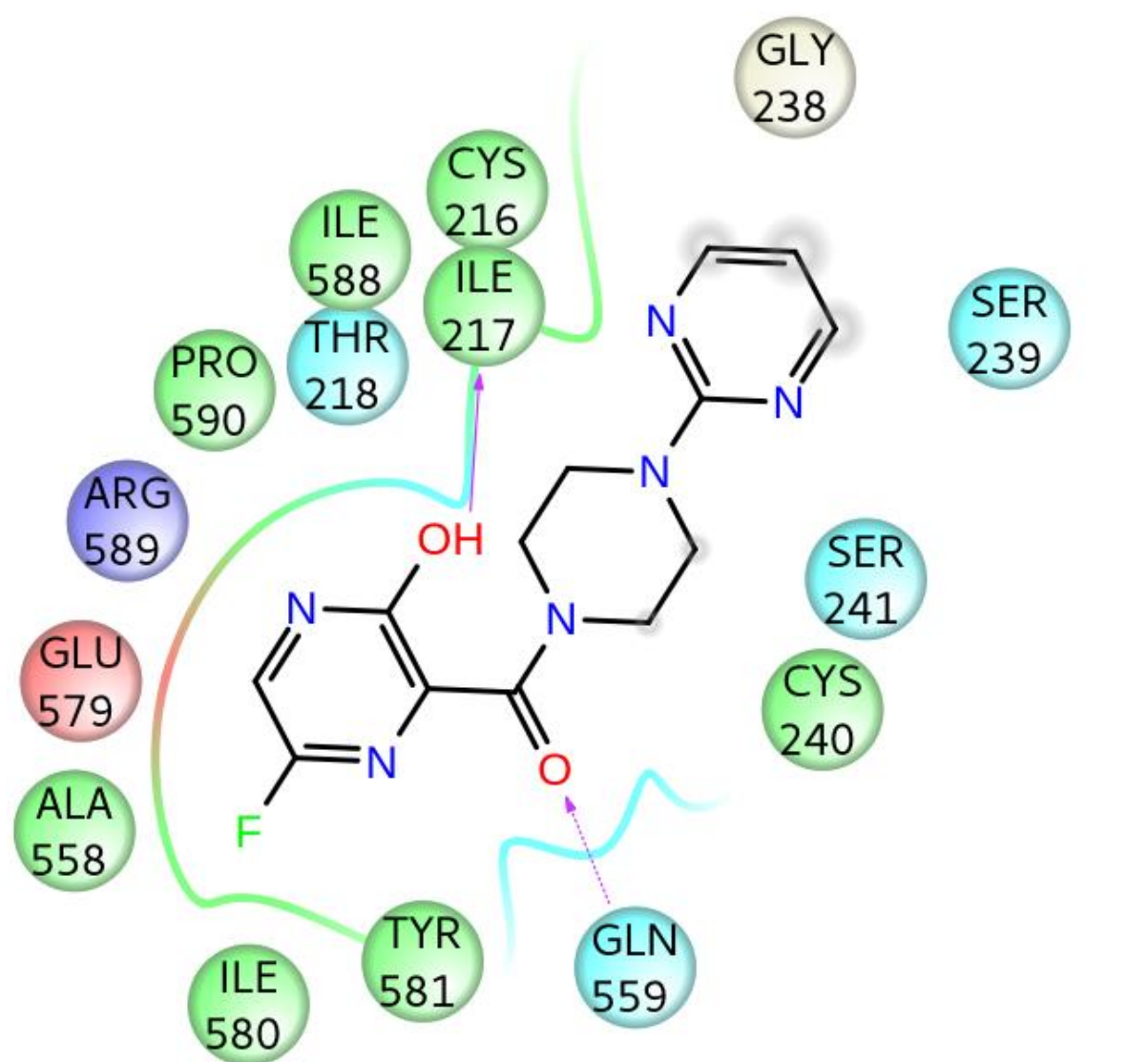
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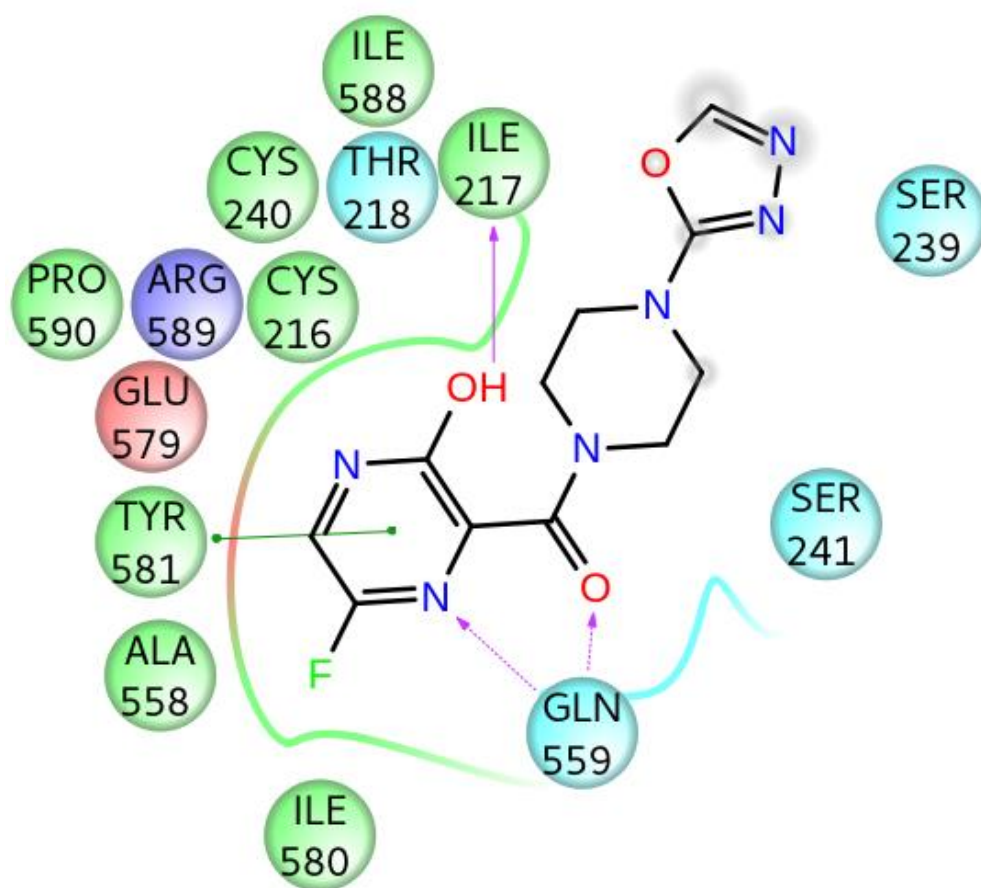
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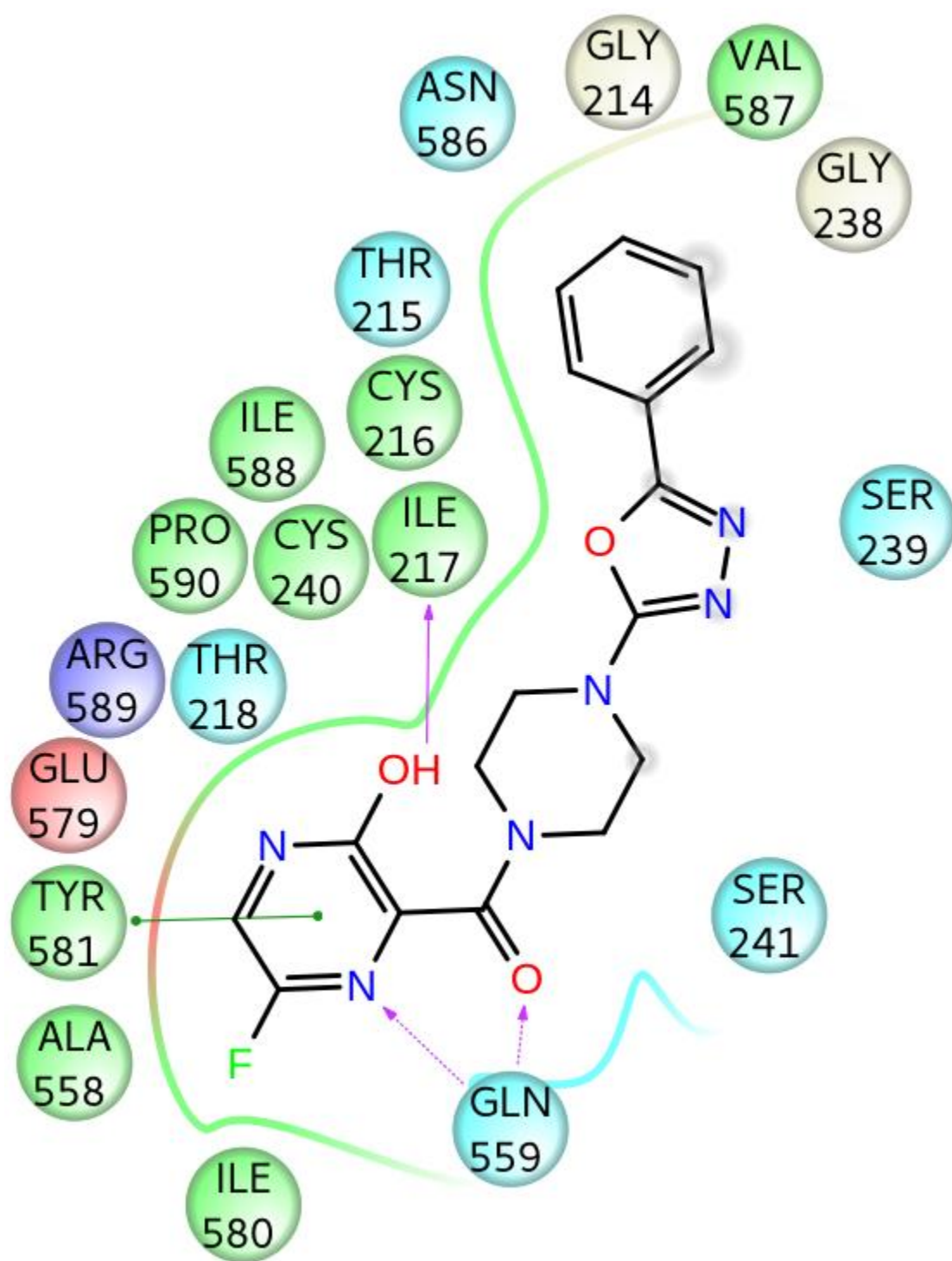
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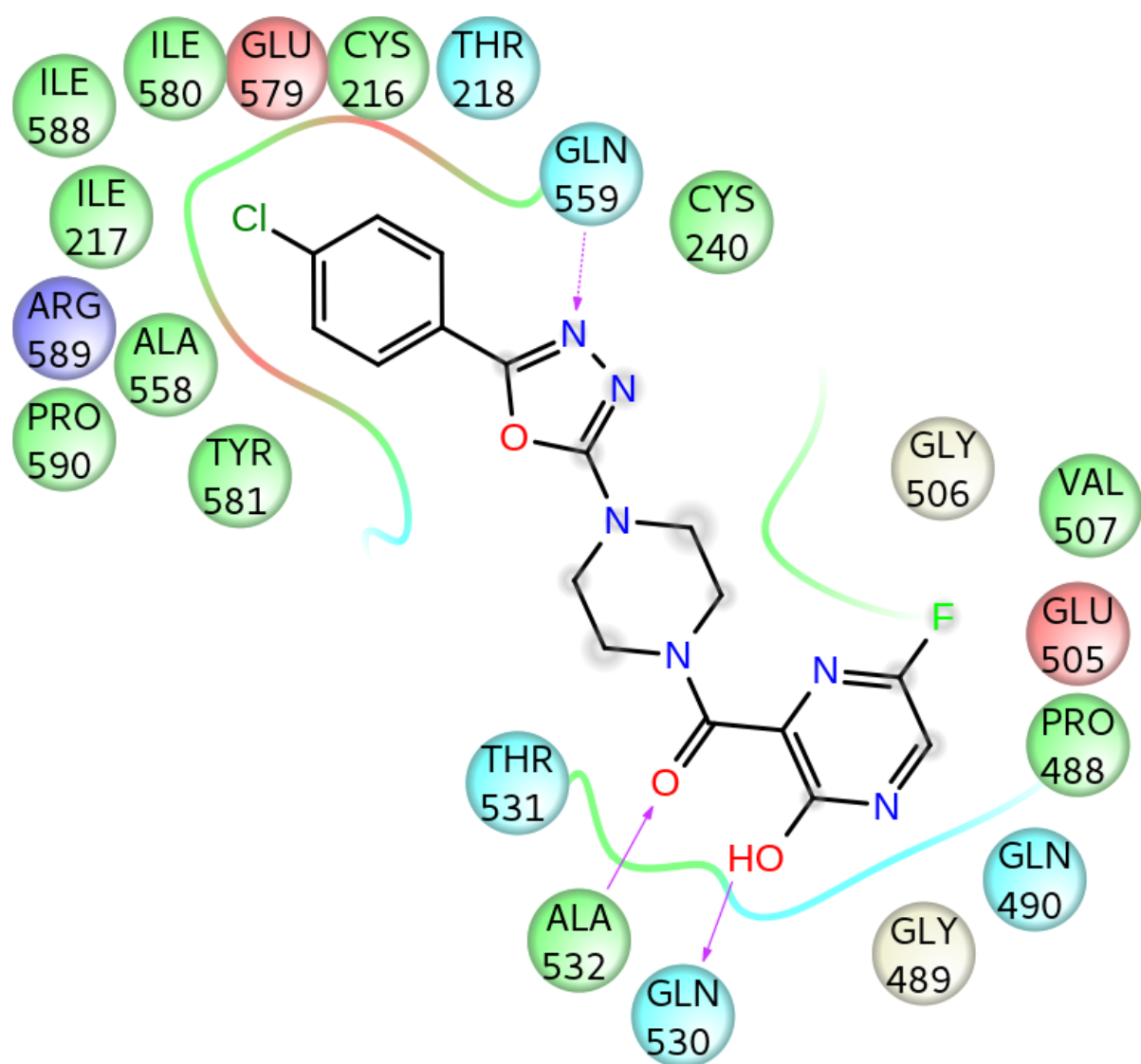
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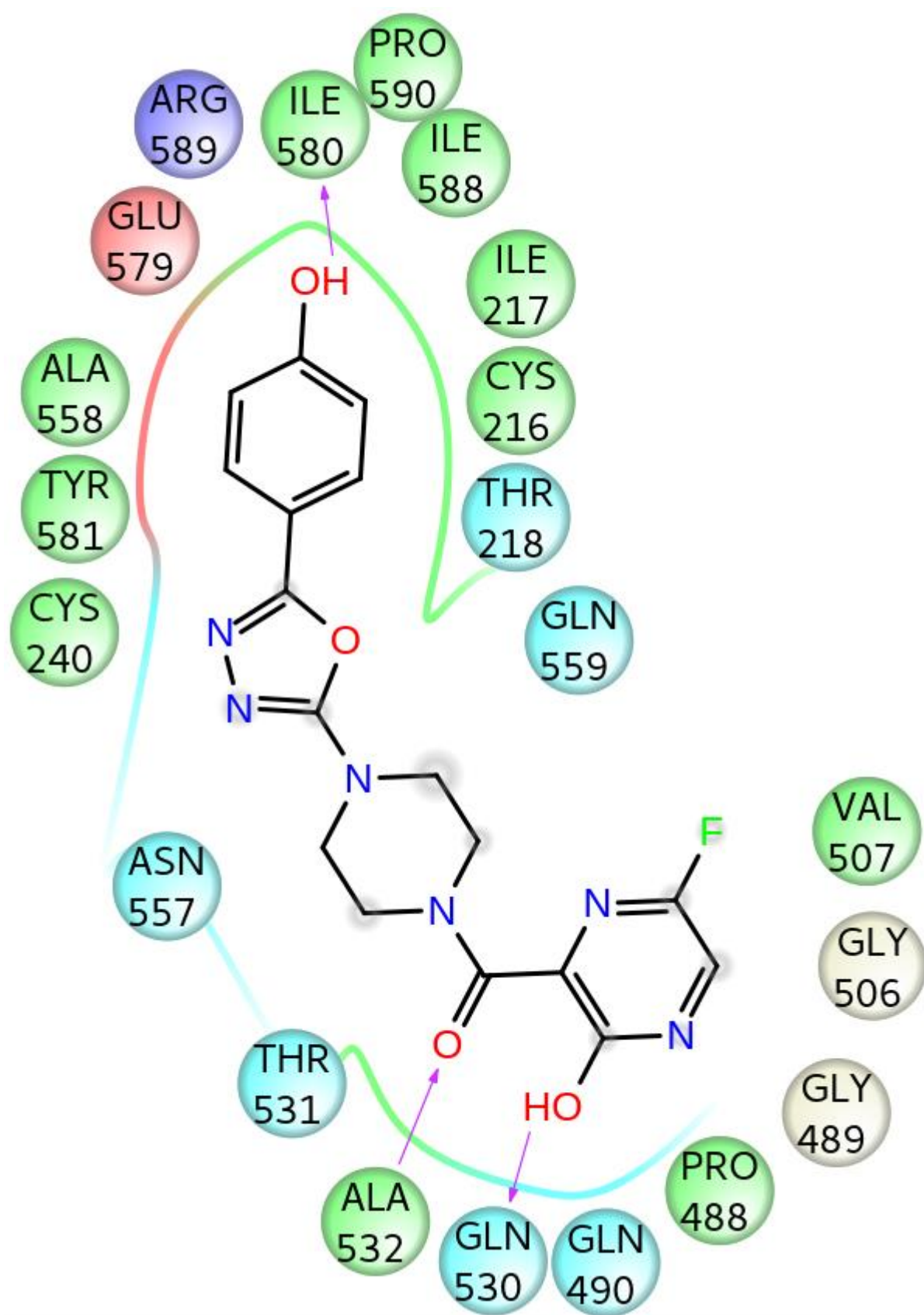
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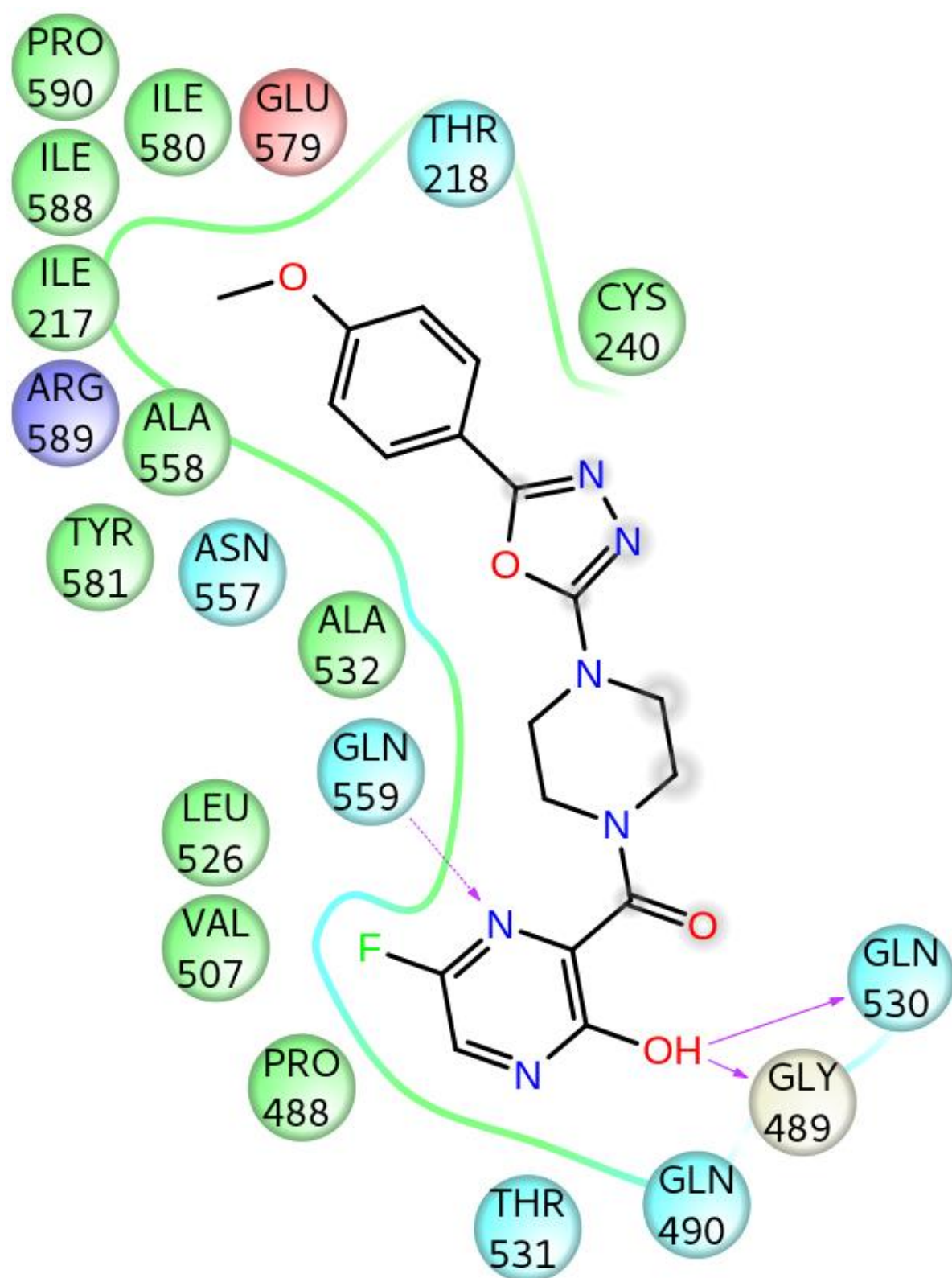
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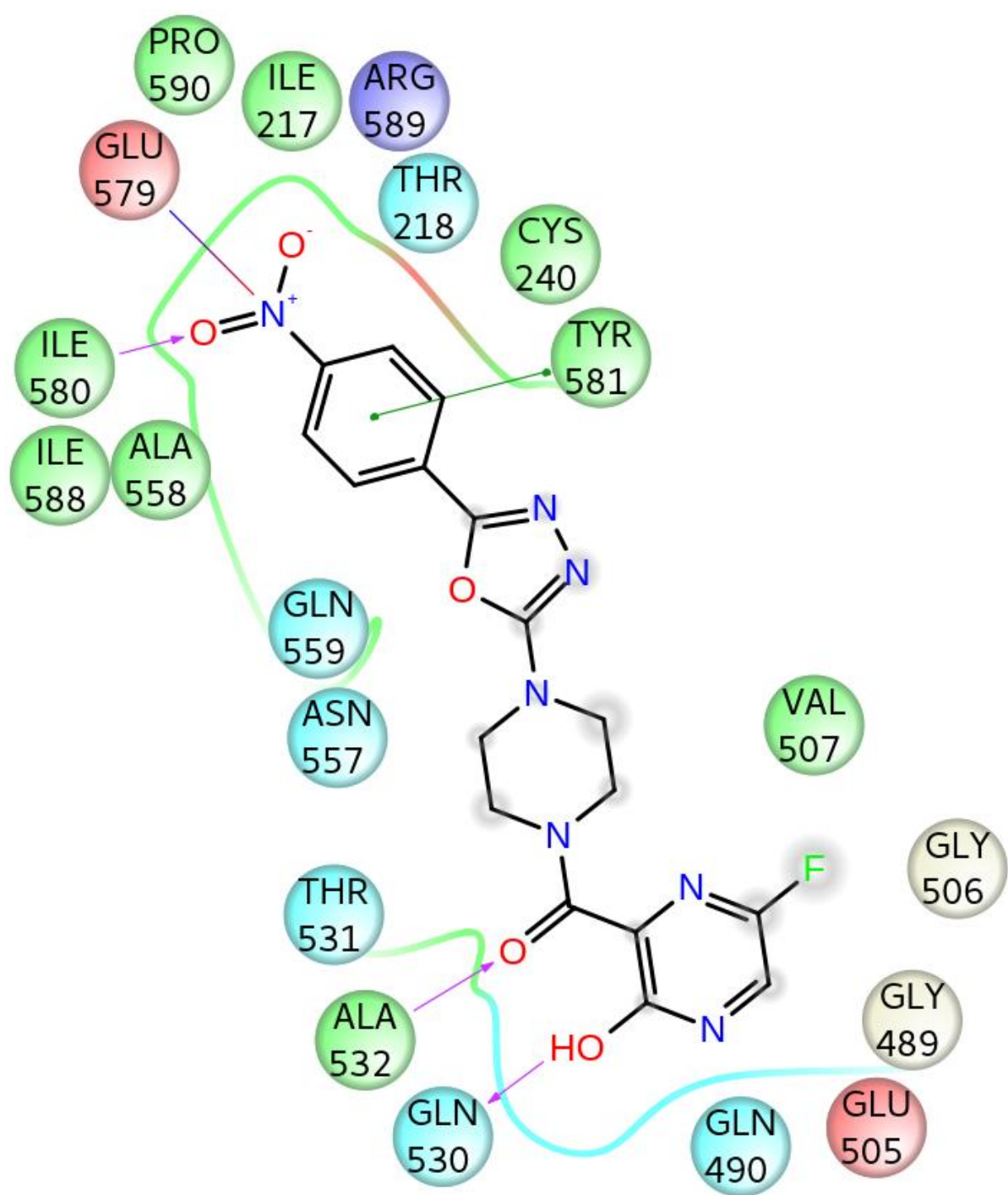
F11



F12



F13



F14